Report on the Workshop for

In-Situ Characterization of Surface and Interface Structures and Processes

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In-Situ Characterization of Surface and Interface Structures and Processes

The workshop on *In-Situ Characterization of Surface and Interface Structures and Processes* was held at the Advanced Photon Source, Argonne National Laboratory on September 8-9, 2005. This cross-cutting workshop brought together experts in synchrotron radiation techniques and various synthesis, processing and modeling efforts to identify future directions in these areas of research; to assess the applicability of x-ray tools to future research problems; and to appraise the interest of the research community in developing dedicated facilities for in-situ x-ray characterization of natural processes and the synthesis, structure and properties of new and technologically important materials at the Advanced Photon Source. Over 130 participants from 39 different research institutions (plus 8 different ANL divisions) representing 16 US States, 8 countries, and 7 synchrotron light sources traveled to the APS to contribute to the talks, poster session and discussion. There were attendees from universities, industry, and from national and international government-sponsored research institutes, representing the broad, diverse interest in this research area.

This workshop was sponsored by the Argonne National Laboratory Advanced Photon Source (APS) and Center for Nanoscale Materials (CNM) as a continuation of the workshop series: *Future Scientific Directions for the Advanced Photon Source & Strategic Planning* that began in August 2004 at Lake Geneva, WI, to contribute to the APS strategic and tactical planning processes. This process has recognized the need for more dedicated and better supported capabilities at the APS. In his charge to the workshop, APS Director J.M. Gibson challenged the participants to identify how the APS could facilitate the best science and growth of the community in this research area. So, this workshop focused on the important surface and interface science enabled by the APS, and also explored how the user community can be strengthened.

1. Introduction & Workshop Scope

Knowledge of atomic and mesoscopic structural arrangements and composition at surfaces and buried interfaces is fundamental to understanding the function and properties of many synthetic structures and reactive interfaces found in nature.

Because of favorable cross sections, x-rays offer a unique opportunity to penetrate through gas, liquid, or solid thin-film overlayers to probe the structure and chemistry of surfaces and internal boundaries from macroscopic lengths down to the atomic level. The brilliance of the APS source enables these in-situ studies, permits real-time investigations to elucidate thin film growth mechanisms, and allows for molecular scale studies of important chemical interactions at internal boundaries. Seminal studies in this area have already been performed at the APS, and this area of research is poised for significant growth.

This workshop successfully brought experts in the area of surface x-ray scattering together with investigators from other fields whose science may benefit from the tools that have been developed (or may be developed) at the APS. In addition, this workshop began to identify the components of an integrated facility that would address important, specific scientific issues in this area, and provide great opportunity for researchers to remain at the forefront of interfacial science.

Some of the research themes in this area are:

- Surfaces, interfaces and nanostructures
- Thin-film growth processes
- Interfaces in catalytic, geochemical and environmental systems
- Electrocatalysts and electrode surface chemistry

The first two topics address controlled growth and characterization of modern materials with nanoscopic to mesoscopic dimensions. These nanostructured materials, notable for their extremely small features, have the potential for wide-ranging applications in diverse fields including energy supply, medical treatment strategies and electronics. Such materials consist of metals, ceramics, polymeric materials, biomaterials or composite materials; and they are often assembled layer-by-layer or even atom-by-atom to generate new atomic arrangements with size-dependent structures and properties. The interplay of confinement, proximity and organization is the key in realizing unique surface and interface properties in these materials resulting in their novel and unpredicted behavior. Understanding and tailoring material synthesis processes to control behavior during growth or assembly, as well as during subsequent processing procedures, are key targets for future research in this area.

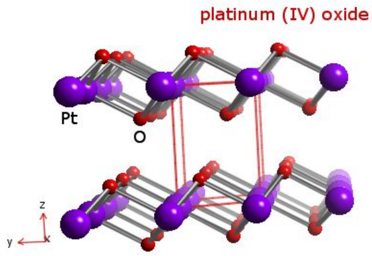
The next two topics deal with chemically active surfaces and interfaces which govern many natural processes in the environment and in technologically important areas, including sensors and fuel cells. Understanding chemical behavior at these surfaces and interfaces is limited by the inability of traditional surface analytical techniques to perform in-situ experiments (for example at liquid-solid interfaces, or at solid surfaces under controlled atmospheres) to measure electronic, chemical, and geometric structures as the catalytic or chemical process progresses.

The topics addressed by the workshop were broad. However the focus was to identify the frontier challenges in understanding changes in atomic arrangement, electronic structure and chemical properties of surfaces and interfaces, both in natural systems and in fabricated structures.

The workshop was divided into scientific sessions that broadly reflected central themes of this research area. These were Growth and Processing (I and II), Complex Interfaces, Frontiers of Interfacial Science, Self Organization, and Real Space Methods. In addition, an Overview session provided perspective of the current state of Interfacial Science worldwide, and established an overall context for the future direction of this research.

2.1 Overview Session

J.F. van der Veen (Paul Scherrer Institut, Switzerland) provided a featured presentation where the rich history of surface science at synchrotron radiation sources worldwide was discussed.

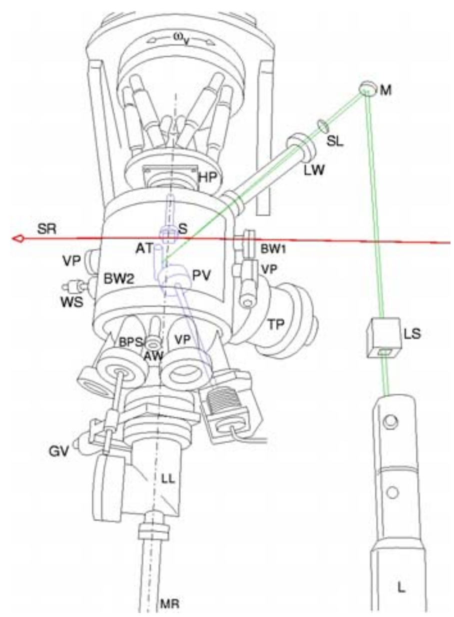


Courtesy: J.W.M. Frenken

Beginning with photoemission spectroscopy using XUV-radiation, the field extended to include a variety of diffraction techniques, exploiting the hard x-ray part of the spectrum. In the 1980's and early 1990's, many researchers simply wanted to know the location of atoms at clean surfaces, and it was discovered that surface reconstructions and accompanying lattice distortions at single-crystal surfaces could be determined by the measurement of CTRs and fractional diffraction orders. These experiments confirmed or falsified theoretical predictions of geometric surface structures. Soon thereafter, these crystallographic studies were extended to buried interfaces. Simultaneously, x-ray standing wave techniques were employed and further developed for the determination of the location of foreign atoms in a host crystal, and for locating specific atomic species at surfaces and interfaces. And, primarily at medium-energy synchrotron sources, angle-resolved photoemission spectroscopy (ARPES) was refined to a very sophisticated level.

Looking to the future direction in this area, the following trends were established as a roadmap:

1. Surface and interface science is becoming increasingly an *applied* science, where one investigates technologically relevant materials and processes. However, the information that is derived from these studies provides new fundamental insights into these systems. In addition, model systems with interesting properties have emerged, such as ordered fullerene layers and step-decorated surfaces.
2. The determination of surface or interface structures is most interesting when the structure is related to the function of the surface or film.
3. Increasing emphasis is being placed on the *in-situ* preparation and analysis of interfacial systems. For example, x-ray diffraction is used to understand the growth process of epitaxial single-crystal oxide films during pulsed laser deposition.

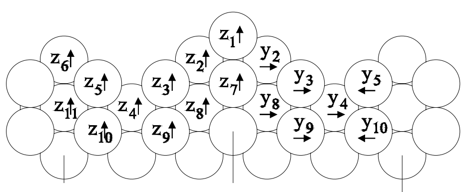


Courtesy: P.R. Willmott

4. There is a shift towards studying samples in more complex in-situ environments as the field has matured. Surfaces are now exposed to a variety of "realistic" conditions, e.g., to a gas mixture at high pressure or to a liquid solution. Such environments more closely mimic conditions present in an industrial catalytic reaction (for example, in a fuel cell) or in the natural environment.

5. Coherent x-ray scattering has a bright future. This technique can be used for the structural characterization (“lensless imaging”) of small objects, deposited clusters, etc. X-ray photon correlation spectroscopy (XPCS) enables us to study, for example, diffusion processes at surfaces.
6. As the synchrotron sources become more brilliant, surface studies in the time domain become possible at ever-faster time scales. This area is expected to go through a revolutionary development with the advent of free electron x-ray lasers.

In another perspective presentation, Ian Robinson (University of Illinois at Urbana-Champaign) presented an overview of the “Uniqueness of Surface Crystallographic Structure Solutions”. He used the example of Pt(110), which is one of the most closely investigated metal surface structures because it displays a variety of “missing-row” reconstructions that are only marginally stable. The ground state is usually found to have 1x2 translational symmetry, but a 1x3 form has also been seen. Between 1x2 and 1x3, a series of disordered structures has been recorded, which shows a slight preference for 1x5 periodicity. Under the preparation conditions used in this study, a stable 1x5 structure was found for Pt(110). Investigation by surface x-ray diffraction led to a complete three-dimensional structure, which closely resembles an alternation of 1x2 and 1x3 unit cells. Pt(110) shows an interesting example of two “homometric” structures that are indistinguishable by diffraction, but are distinguishable by virtue of their subsurface relaxation pattern. The importance of identifying non-unique solutions of surface structures was discussed.



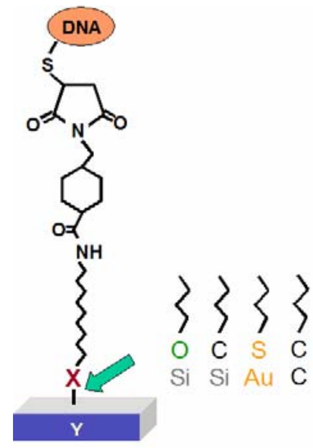
Courtesy: I.K. Robinson

2.2 Frontiers of Interfacial Science

At the session on *Frontiers of Interfacial Science*, there were presentations that included both characterization of fabricated systems, and studies of natural interfacial systems.

For example, tribological processes that influence friction and wear involve a complex combination of materials science, physics, chemistry, and rheology. The understanding of sliding contact phenomena is limited by the fact that these interactions take place at buried interfaces. Most often the only evaluation of these interfaces is accomplished through *ex situ* means after separating the contacts. *In-situ* approaches to studying friction and wear processes are challenging because most engineering surfaces are metals or ceramics that have no optical transparency at visible wavelengths. For this reason, most of what is known to date about interfacial processes occurring during sliding has been learned through optical probes of bearing interfaces. In her presentation, Kathryn Wahl (US Naval Research Laboratory, Washington, DC) presented examples of the kinds of physical and chemical processes occurring in buried sliding interfaces. Film thickness, chemistry/phase, rheology, morphology, and contact pressure are readily determined by optical methods. These real-time, *in-situ* methods show a rich variety of materials processing phenomena that occur during sliding, and have demonstrated that steady state friction values often correlate with interface chemistry, while dynamic instabilities are associated with morphology changes. It is clear that the scientific issues and opportunities for advancing our understanding of interfacial phenomena in tribology can benefit from techniques (such as hard x-ray scattering and imaging tools) that penetrate to the buried, sliding interface.

The *Frontiers of Interfacial Science* also included highlights where organic and hierarchically assembled inorganic/organic hybrid films are featured. For example, while microelectronics has largely revolved around the use of inorganic materials such as silicon, advances in emerging fields such as biotechnology and nanotechnology are often based upon organic and/or biological materials. Diamond and other forms of carbon are particularly interesting because of their high degree of chemical and thermal stability. However, chemical modification of diamond remains relatively unexplored. In his presentation, Robert J. Hamers (Univ of Wisconsin, Madison, WI) discussed new methods for functionalizing surfaces of diamond, gallium nitride, and other wide-gap semiconductors, demonstrating that the interaction with biomolecules can be precisely tailored via surface chemical modification and that these materials can be used to make bio-electronic devices such as biologically sensitive field-effect transistors. There are many questions that remain unanswered about the nature of these interfaces, particularly when two or three chemical steps are required, and synchrotron-based methods may be able to provide important insight into these issues.

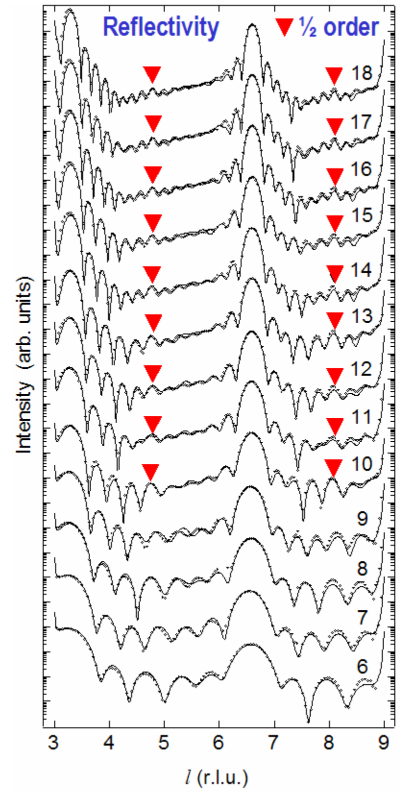


Courtesy: R.J. Hamers

The formation, physical characterization, dynamical properties, and reactivity of thin films are central to our understanding of interfacial science, including nanoscale systems. In his presentation, Steven Sibener (University of Chicago, Chicago, IL) focused on the characteristics of organic and hierarchically assembled inorganic/organic hybrid films, in free thin films as well as under nanoscale confinement. Beginning with a discussion of issues pertaining to defect mobility and thermal annealing, the spatial organization, and the prospect for functional decoration of diblock copolymer surface structures was presented. This effort demonstrated that atomic force microscopy imaging can be used in a time-lapse manner to track the interactions of topological defects. Strong polymer alignment was realized in dewetted annular structures and on lithographically generated grating substrates in which intentionally selected depths and widths were used to guide the assembly of highly aligned polymeric interfaces under either kinetic or thermodynamic control. The phase-separated 25-nm diblock cylinders geometrically aligned by this procedure are essentially defect free, exhibit remarkable spatial coherence spanning microns, and are structurally compliant as is characteristic of "soft" organic systems. This presentation also described experiments that use elastic/inelastic neutral atom scattering to probe the surface structure/molecular dynamics of self-assembling monolayers (SAMs) and polymeric thin films. These measurements are important as they characterize the atomic-level surface vibrational dynamics of thin films and polymers. Such measurements also probe how the properties of nanoscale thin films may differ from those characteristic of bulk materials.

2.3 Self-Organization

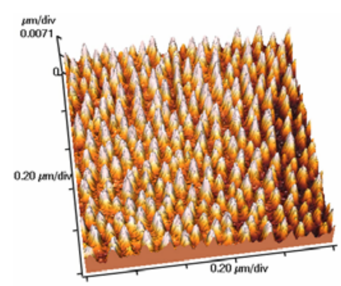
The issue of confinement effects was more thoroughly examined in the *Self-Organization* session where the presentations carefully considered the effects of size (confinement), strain, composition, and defect structures.



Courtesy: T.C. Chiang

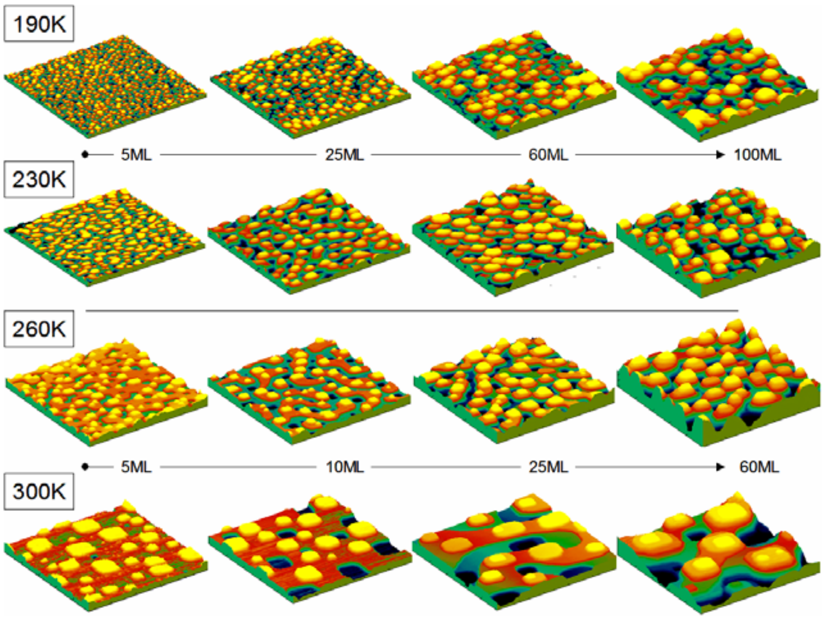
Tai Chiang (University of Illinois, Urbana-Champaign, IL) spoke about metal films on semiconductor substrates that exhibit interesting growth behavior, structure, and properties as a result of quantum confinement of the valence electrons in the films. He discussed three related experimental observations. In the first case, quantum confinement leads to Friedel-type charge oscillations and a corresponding lattice distortion, which can be detected by x-ray diffraction. In the second case, quantum confinement results in large oscillatory variations in the system total energy as a function of thickness. As a smooth film is annealed, it develops a thickness distribution that reflects the energetics of the system. The “roughness” of the annealed film is actually highly structured. In the third case, thin film growth at temperatures where diffusion occurs readily can exhibit unusual behavior, including the formation of magic height islands. In these examples, the application of hard x-ray scattering and diffraction techniques provides insight into the understanding of structural phenomena that are dictated by non-classical effects in thin film systems.

Chia-Hung Hsu (National Synchrotron Radiation Research Center, Taiwan) discussed how the size, shape, strain distribution, compositional profile and spatial distribution are the critical factors that determine the electronic level and thus the physical properties of semiconductor nano-structures. For MBE-grown quantum dots and quantum wires, lattice mismatch, surface segregation, interface diffusion and various kinetic effects make their formation mechanism very complicated. In fact, the structure and the formation mechanism of these self-assembled nano-structures are still not well understood. In this work, grazing incidence x-ray scattering methods including reciprocal space map and small angle x-ray scattering were applied to study the strain field, shape and spatial distribution of III-V semiconductor nano-structures. In particular, focus was placed on the application of resonant x-ray scattering techniques to determine the compositional distribution within the nano-structures and its correlation with strain field.



AFM image of self-assembled $In_{0.5}Ga_{0.5}As$ QDs on GaAs(001) surface. (Courtesy: C-H. Hsu)

Homoepitaxy provides an ideal testing ground for fundamental concepts and understanding of thin film growth. Jim Evans (Iowa State University & Ames Laboratory, Ames, IA) presented some of his work on integrated modeling and experimental studies of homoepitaxial thin film growth. Despite the relative simplicity of these systems, unexpected behavior continues to emerge, due in part to the feature that deposition drives the morphology and structure of the growing film far from equilibrium. The most significant recent advances have often come from integrating experimental and modeling studies, incorporating key experimental data into the development of atomistic models which then have quantitative predictive capability.

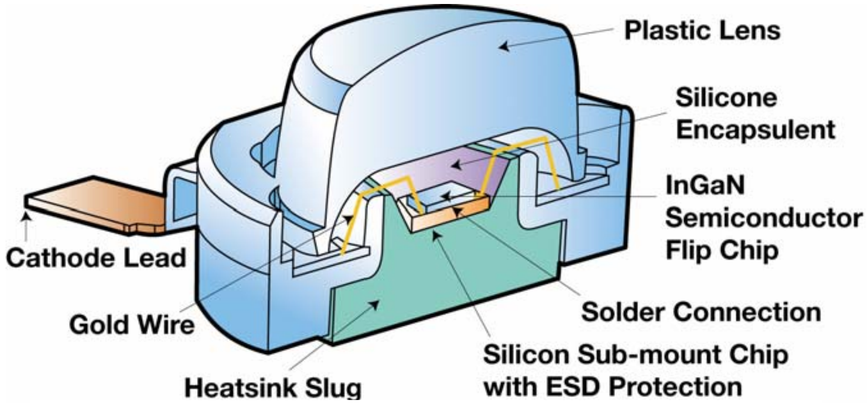


Courtesy: J. Evans

The initial stage of homoepitaxial growth involves the formation of single-atomic-layer-thick two-dimensional islands on the substrate (due to the diffusion-mediated aggregation of deposited atoms). Subsequently atoms are deposited on top of existing islands, producing multilayer stacks of two-dimensional islands or “mounds” (due to inhibited downward transport at island edges). Surface x-ray diffraction (XRD) and STM have been applied to study both regimes, focusing on the multilayer regime, where the diffraction technique is particularly useful in characterizing “kinetic roughening” of the growing film as well as the subtle dynamics of “mound coarsening”. In addition, due to its sensitivity to strain, surface x-ray diffraction provides an invaluable tool to probe the incorporation of internal vacancies or voids, recently discovered in growing homoepitaxial films.

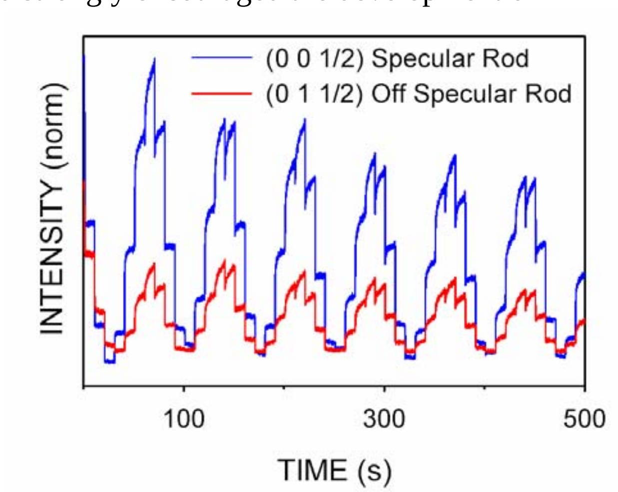
2.4 Growth and Processing I & II

A strong and vibrant community working on *in-situ* analysis of crystal growth, thin film structure and processing of materials has developed over the last ten years at the Advanced Photon Source. A few representative studies were discussed, demonstrating the wide-ranging importance of the research being conducted at the APS in this area, and pointing at new directions that hold promise for critical discovery.



Cross-section view of Luxeon emitter (courtesy: A. Munkholm)

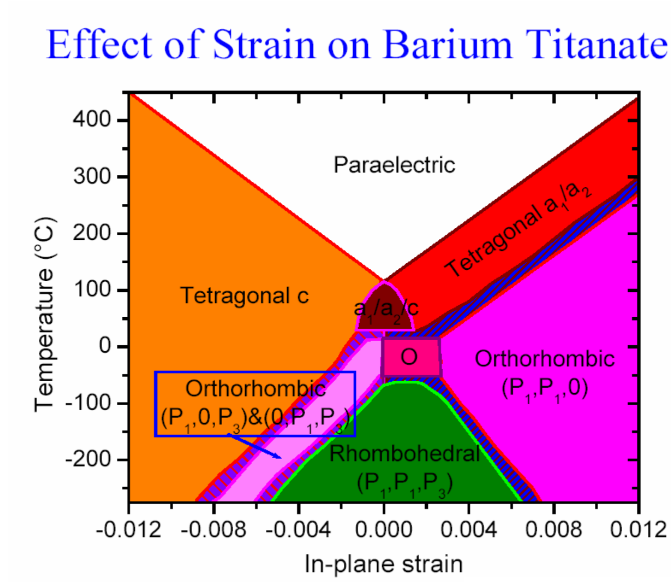
Anneli Munkholm (Lumileds Lighting LLC, San Jose, CA) discussed the importance of LED lighting in the energy future of the Nation. High-efficiency LED lighting could reduce the global electricity usage by 10% saving $100 billion in costs and eliminating 200 million tons of carbon emissions per year. The development and production of LEDs for lighting applications is critically dependent on understanding the growth of GaN and related materials. Since these materials are typically grown by metal-organic chemical vapor deposition (MOCVD) at high ambient pressure and temperature, in-situ x-ray scattering has proven to be a crucial technique for monitoring the process. In particular, the MOCVD system at the APS has been used to understand the effect of silicon dopants on the growth. In recent experiments, the use of total reflection x-ray fluorescence (TXRF) measurements along with GIXS during growth determined that indium condensation was playing an unexpected role in the growth of InGaN, a key material in solid-state lighting. Dr. Munkholm emphasized that research at the APS has the potential to significantly contribute to deeper understanding of InGaN growth and strongly encouraged the development of more facilities to enable this research.



G. Eres, J.Z. Tischler, M. Yoon, B.C. Larson, C.M. Rouleau, D.H. Lowndes, and P. Zschack, Appl. Phys. Lett. 80, 3379 (2002)

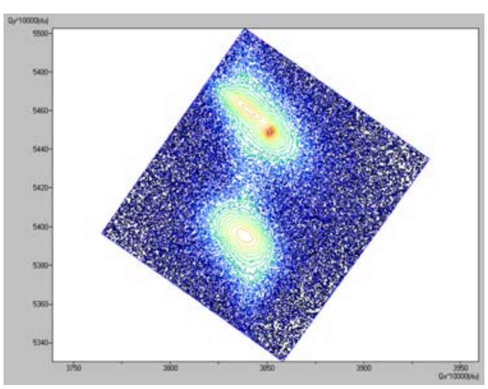
Pulsed laser deposition (PLD) is a powerful technique for developing new materials and is widely used in research labs around the country. Oak Ridge National Laboratory researchers have developed capabilities at the APS to study the basic materials physics of PLD and to optimize processing techniques and critical growth parameters. Gyula Eres (Oak Ridge National Laboratory, Oak Ridge, TN), described this facility and discussed pioneering research into PLD growth of homoepitaxial $SrTiO_3$. Of particular note is the window that PLD offers into microsecond and nanosecond dynamics of structural rearrangements on surfaces. This unique capability offers deep insight into the fundamental atomic mechanisms of growth.

Darrel Schlom (Pennsylvania State University, University Park, PA) has been performing studies of complex oxides and the integration of complex oxides into semiconductors both in his lab at Penn State and at the APS. These complex oxides have a wide variety of important properties since they are ferroelectrics, ferromagnets, ferrimagnets, multiferroics, superconductors, colossal magnetoresistors and semiconductors. The flexible incorporation of these materials into electronic devices would enable a wide range of new and enhanced functionalities. However, use of these materials requires a much better understanding of the underlying physical mechanisms controlling growth and better ability to control composition. Prof. Schlom identified two grand challenges that *in-situ* analysis at the APS is ideally suited to address: 1) composition measurement and control to the 100 ppm level in ultra-thin films during growth and 2) developing a detailed knowledge of interface evolution (including buried interfaces) during processing. In this last area knowledge of the average structure, the chemical and electronic structure (e.g. oxidation state), and the imaging of defects at the interface are all important and accessible using x-ray synchrotron techniques.



Courtesy: D. Schlom

James Harris (Stanford University, Palo Alto, CA) brought a long-term and deep perspective to the growth of high-quality semiconductor structures. He described a program that his group has been pursuing for a number of years into the growth of novel opto-electronic materials including GaInNAsSb films and Ge/SiGe quantum wells. In these systems, the combination of composition, strain and three-dimensional shape is used to create materials of unique optical and electronic properties. However, traditional characterization techniques have great difficulty in characterizing these complex materials. Prof. Harris identified several areas and techniques where *in-situ* x-ray techniques could make very important contributions including:



Courtesy: J. Harris

- Reciprocal Space Mapping (RSM) of the materials at a much higher rate and with much greater sensitivity. The enhanced sensitivity can identify minor phase segregation and clustering which can significantly impact device performance. It can also measure interfacial quality during and after processing steps.
- Grazing incidence scattering to determine film quality.
- High resolution topography to measure dislocations
- X-ray spectroscopy to measure the complex electronic structures and chemical properties of these materials.

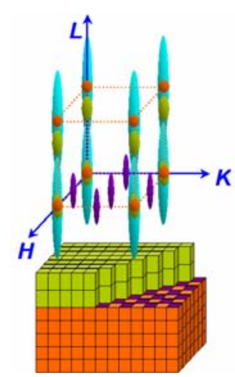
Prof. Harris emphasized the need to do these measurements on a single sample and in real time to identify where and when structural and electronic transformations occur. Without such knowledge, developing robust production technologies is very difficult.

A research field of great promise is the self-assembly of nanostructures to create materials with exceptional properties. Robert Hull (University of Virginia, Charlottesville, VA) described a systematic research effort aimed at directing self-assembly to create quantum cellular automata and other novel devices. In their research, a focused ion beam (FIB) is used to modify the surface locally with a pre-determined pattern. This pattern then influences the nucleation and self-assembly of quantum dot molecules (QDM) to create a highly ordered array of QDM's. Strain, wetting layers and composition can be used to create QDM's with unique shapes and properties. Prof. Hull discussed a series of open questions including the following:

- How is the information for self-assembly most effectively encoded.
- What are the energetics, length scales and time scales of self-assembly?
- What is the best metric for the magnitude of information encoded in the surface?
- What degree of precision in nanoscale assembly, controlled impurity/dopant incorporation is required?
- How complex a pattern can be encoded in the surface?

He then identified a particularly promising approach to these problems as being the use of in-situ x-ray diffraction studies coupled with the existing surface modification and growth techniques being used in his group (e.g. FIB and TEM).

While there is a very robust program on growth of materials at the Advanced Photon Source, the effort into the subsequent processing of these important thin film materials is less mature. Karl Ludwig (Boston University, Boston MA) discussed the XSMART (X-ray Studies of Materials with Analysis in Real Time) program that he and Prof. Randall Headrick (University of Vermont) have developed at the NSLS. This program is investigating surface evolution and nanostructure development during ion bombardment and plasma processing. Prof. Ludwig presented two specific examples of the types of problems being studied. First, x-ray scattering has proven very useful in monitoring the development of nanostructures on the surface of GaSb during low energy (500 eV) ion bombardment with Ar. In this case, grazing incidence x-ray scattering was used to probe the size of the nanostructures, the long-range correlations present on the surface and the strain state of the resultant nanodots. Similar techniques were used to study the evolution of sapphire surfaces during plasma-assisted nitridation (a key step in the growth of GaN thin films which are important for solid state lighting). Since detailed x-ray measurements can be obtained in real time, they can be used to test theories and simulations predicting the time-evolution of the surface structures in both of these cases.



Courtesy: D. Fong

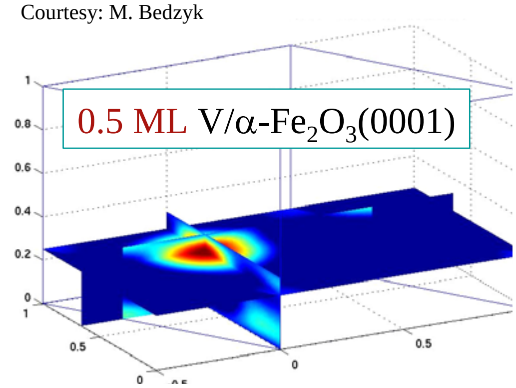
The final processing area covered dealt with in-situ oxidation and chemical processing measurements of metal surfaces and thin films. Dillon Fong (Argonne National Laboratory, Argonne, IL) described the results of measurements performed at the APS. Oxidation of metals is, of course, a highly studied problem in the bulk. However, as we seek to exploit the unique chemical and electronic properties of nanostructures, the chemical properties of very thin films and small islands becomes a focus of attention.

In the work Dr. Fong described, thin (200 nm) thick copper films were deposited on $SrTiO_3$ substrates. The initial stage of oxidation of these films was studied using grazing incidence x-ray scattering under near equilibrium conditions. By studying the oxidation under carefully controlled partial pressures of reactant gasses, Dr. Fong and coworkers were able to map out the equilibrium phase boundary between Cu(001) films and Cu_2O nanoislands. They found this phase boundary to be orders of magnitude higher than that predicted based on bulk thermodynamics. This work demonstrates the usefulness of *in-situ* structural measurements for understanding the behavior of nanostructures in an elevated temperature, controlled atmosphere environment. Dr. Fong described ongoing efforts to extend these capabilities into both the fundamental science of oxidation and into new areas such as the catalytic activity/structure relationships of nanoparticles.

2.5 Real-Space Methods

Interfacial scattering methods, as traditionally practiced, are impeded by the crystallographic phase problem. Simply stated, the scattering intensity measured in the far field is proportional to the square modulus of the structure factor, which in turn is the Fourier transformed electron density. Phase information is lost in x-ray scattering measurements in the far field. Various advances have begun to make use of the fact that the phase information can be obtained in many cases. This allows real-space electron density (with Å – scale resolution) to be obtained directly from the data, thereby effectively transforming x-ray scattering into an imaging approach with excellent spatial sensitivity.

Courtesy: M. Bedzyk

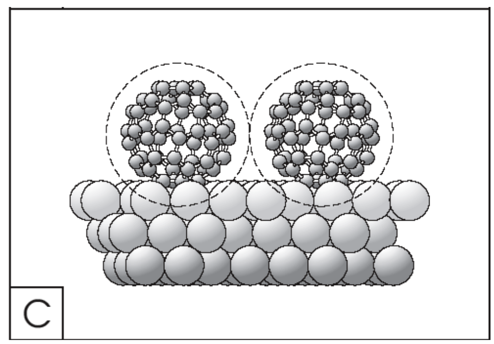


X-ray standing waves has long been known as a phase-sensitive technique, since the measured x-ray fluorescence probes the electric field intensity near the interface (i.e., in the near-field). Michael Bedzyk (Northwestern University, Evanston, IL) described how this phase-sensitivity of XSW could be used to probe complex reactions at solid-vacuum and solid-liquid interfaces. In particular, the direct use of measured phases leads to the ability to create real-space images without reference to model structures (x-ray standing wave imaging). The use of x-ray fluorescence also leads to elemental specificity, which is important for complex interfaces. Examples include measurements of oxidation state driven changes in catalyst structures, epitaxy of integrated oxide materials on semiconductor surfaces, molecular nano-patterning of organic based molecular structures on silicon, and polyion condensation at charged liquid-solid interfaces.

Recent advances in interfacial x-ray scattering are beginning to make use of theoretical concepts revealing that lost phase information can be recovered from diffraction data measured in the far field, thereby bypassing the phase problem. One approach to recover lost phase information is by "oversampling", originally developed in the context of coherent scattering from micron-sized particles. Paul Lyman (University of Wisconsin, Milwaukee, WI) described how these ideas could be applied to the continuous crystal truncation rods of interfacial scattering, providing the first demonstration that phase information of interfacial diffraction data can be extracted using error correction algorithms so that interfacial structures can be imaged without reference to model structures (and ultimately guide the final quantitative model-dependent optimization). Here the clean structures of Au(110) and surface alloy phases for various Sb coverages were determined.

Yizhak Yacoby (Hebrew University, Jerusalem, Israel) described a different approach to image thin film structures, by making use of the slowly varying structure factor of the thin film (e.g., the CoBRA method) and the known substrate (reference) structure which allows the phases to be estimated so that the interfacial structures can be obtained. This approach was applied to oxide thin films ($PbTiO_3$/$SrTiO_3$, and Gd_2O_3/GaAs) where various aspects of the film structure were determined, including interfacial strain displacements, stacking order. Extensions of this approach to probe the surface structures of organic molecular crystals were described.

Courtesy: R. Felici



The application of direct methods approaches to interfacial crystallography concepts was highlighted by Roberto Felici (Instituto Nazionale per la Fisica della Materia – OGG, ESRF, Grenoble, France) for the case of fullerene (C60) adsorption on metal surfaces. These interfacial structures consist of changes in the substrate lattice as well as the associated fullerene adsorbate structure. The case of C60 on Au(110) showed a reconstruction whose structure was solved with the direct methods approach. The case of fullerenes on Pt(111) was not amenable to this approach, which was instead solved by using the heavy atom method applied to vacancy distributions in the Pt substrate, ultimately providing sensitivity to the C60 location and orientation.

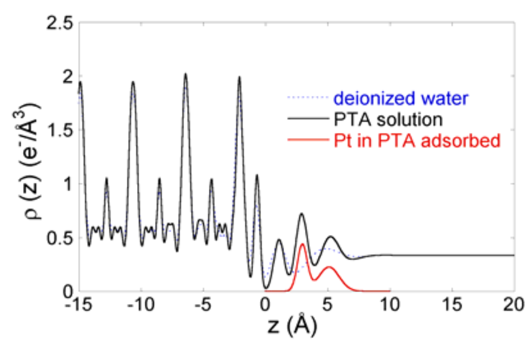
These presentations highlighted important new approaches for understanding interfacial scattering data. These approaches, and other ongoing developments in this area, lead to an ability to obtain a direct first-order model independent analysis of data, thereby eliminating the most labor-intensive step in structural analysis.

2.6 Complex Interfaces

Interfacial reactivity is central to many areas of science and technology. “Real” interfaces are found in ambient or aqueous environments and present significant challenges due to various structural and compositional complexities. The ability to understand such interface has been limited until recently, where measurements of model systems with essential added degrees of complexity.

Gordon Brown (Stanford University, Stanford, CA) reviewed the current state of understanding of complex geochemical interfaces found in nature that control the fate and transport of contaminants, where essential degrees of complexity include speciation, surface reactions, natural organic matter coatings, microbial biofilms, and nanoparticles. The importance of defects and surface termination was revealed by the hydroxylation of MgO, Al_2O_3 and Fe_2O_3 surfaces, and the influence of model biofilms on substrate reactivity was also studied with long period x-ray standing waves. The importance of heterogeneity at interfaces was discussed and probed using soft x-ray microscopy. Soft x-ray scanning transmission x-ray microscopy studies of microbes bound to surfaces revealed changes to the elemental distribution and speciation surrounding the microbe at the sub-micron scale. The ability to probe electron transfer reactions during biomineralization was established using current sensing atomic force microscopy. The potential human health impact of these phenomena was highlighted with the recent tragedy in Bangladesh due to arsenic contamination in the ground water and its relationship to soil constituents.

The use of resonant anomalous x-ray reflectivity for interfacial studies was discussed by Changyong Park (Argonne National Laboratory, Argonne, IL). Here the reflectivity as a function of photon energy is used to obtain element specific structures, as well as revealing spectroscopic sensitivity of interfacial species, both in an interface specific manner. Results on relatively simple examples derived from geochemical systems and catalyst preparation illustrated these capabilities. Extensions of this capability that were discussed include the ability to obtain model-independent elemental profiles and its use as a probe of ion adsorption equilibria.



Courtesy: C. Park

The inter-relationships of structure and catalytic activity at electrified metal-aqueous interfaces were discussed by Nenad Markovic (Argonne National Laboratory, Argonne, IL). X-ray scattering was used to delineate the interfacial structure as a function of electrochemical potential, solution composition (e.g., carbon monoxide) and temperature, with complimentary information from other approaches including FTIR. These results demonstrated the important changes in interfacial behavior (both thermodynamics and kinetics) for relatively small changes of temperature, the competitive adsorption of CO and OH, and the coexistence of structures, necessitating a comprehensive understanding of the fundamental reactions.

Together these presentations highlighted some of the challenges that must be met to understand reactions at real interfaces, with examples ranging from geochemistry to microbiology to catalysis. Specific examples highlighted the unique insights that can be obtained from synchrotron-based approaches, especially when coupled with complimentary approaches, including imaging and spectroscopy.

2.7 Outlook

This workshop highlighted the broad range of current and potential activities in the area of *In-Situ Characterization of Surface and Interface Structures and Processes* being performed primarily using x-ray scattering techniques. These activities have had significant impact in diverse fields such as semiconductor processing, catalysis, and geochemistry. A compelling vision of their evolution into new areas of materials science, environmental science, chemistry, nano-scale physics, and materials processing was presented during the two day workshop, and speakers were unanimous in their view that these techniques have great impact on fundamental problems in basic and applied sciences.

This perspective was recently reinforced in a special issue in Nature dedicated to Surfaces and Interfaces [Nature, **437**, 29 September 2005]:

> *The importance of interfaces cannot be overestimated. They play a vital role in technological applications as diverse as catalysis, microelectronics, lubrication, corrosion, photography and in many environmental processes… Although their significance has been realized for centuries, surfaces and interfaces long evaded detailed scrutiny at the atomic scale…As our understanding of these peculiar regions of matter grows, along with the range of characterization and manipulation tools at our disposal, we are in a position to use the unique environment of surfaces and interfaces to explore fascinating science and new applications.*

Progress in the field of integrated materials assembly, processing, and characterization is intimately related to the achievements in the development of dedicated *in-situ* analytical techniques that enable us to examine the atomic and electronic structure of materials, and unravel and quantitatively analyze physical, chemical and biological phenomena and processes. Hard x-ray scattering, spectroscopy and imaging tools are capable of delivering monolayer resolution with the greatest chemical sensitivities and ultimate detection limits, along with capabilities for *in-situ* and non-destructive analysis. Numerous workshop presenters argued that application of these x-ray techniques in their field would lead to breakthroughs in scientific and technological problems. Presenters also argued that a facility which combined increased availability of these x-ray techniques with ready access to traditional techniques such as electron microscopy would greatly accelerate progress. In a new paradigm in which all these *in-situ* techniques become available at one integrated materials creation and characterization facility, there are unprecedented opportunities for progress in the understanding and creation of new materials, and understanding natural phenomena at internal boundaries.

Progress in interfacial chemistry (including geochemical and environmental processes, electrochemistry, fuel cells, and catalysis) often requires distinct approaches due to the emphasis on solid-liquid interfaces and the inapplicability of electron based approaches. In this area, x-ray scattering techniques provide unique information about interfacial structure and processes through direct, in-situ, and real-time observations that cannot be obtained in any other way. Here, the use of element specific approaches is also often necessary, which invariably involves tuning or scanning the photon energy to highlight particular aspects of the interfacial structure (e.g., resonant scattering, x-ray standing waves).

The APS, the collocated Center for Nanoscale Materials (CNM), and the supplemental resources of Argonne National Laboratory provide a unique environment for pursuing this vision. They provide state-of-the-art facilities in x-ray science, materials synthesis and fabrication, electron microscopy, and many other relevant techniques. The challenge going forward is to leverage these capabilities into an integrated effort that enables researchers to use their sophisticated expertise to tackle these important scientific and technological problems in a timely, efficient and productive manner.

3.1 Overview of current capabilities at the APS

The Surface and Interface Scattering capabilities for in-situ studies that have been developed at the APS are a result of the scientific leadership and investments of traditional Collaborative Access Teams (CATs). Seven different CAT groups have developed these capabilities in 9 different APS sectors. An impressive suite of instruments and capabilities have been developed at the APS and are widely distributed around the ring.

These capabilities fall into three general categories. The first is Special Purpose instrumentation where the x-ray capabilities are integrated into the experimental apparatus. These are represented by the large, dedicated growth chambers (MBE, MOCVD, PLD, etc..) that are usually stationery in an experimental hutch. The experimental hutches for these instruments often require extensive upgrades to provide the necessary support (e.g. safety) systems. The second category involves specialized reaction chambers or cells that attach to general-purpose diffractometers, and often involve elaborate ancillary gas handling or processing equipment. The third category is General Purpose scattering, where a sample or small sample cell is mounted to a general-purpose diffractometer for ex-situ characterization and study. The first two categories of instruments require extensive floor space for their associated support infrastructure.

Sector	Special Purpose Systems	Specialized Chambers	Ex-situ Related Studies	Total Usage
5 ID	0.05	0.09	0.07	0.2
6 ID	0.14			0.14
7 ID		0.04	0.24	0.29
11 ID		0.48		0.48
12 ID	0.39	0.27		0.67
13 ID		0.29		0.29
20 ID	0.20		0.13	0.33
33 ID	0.34		0.08	0.42
34 ID	0.27	0.14		0.41
			Total Usage	3.2

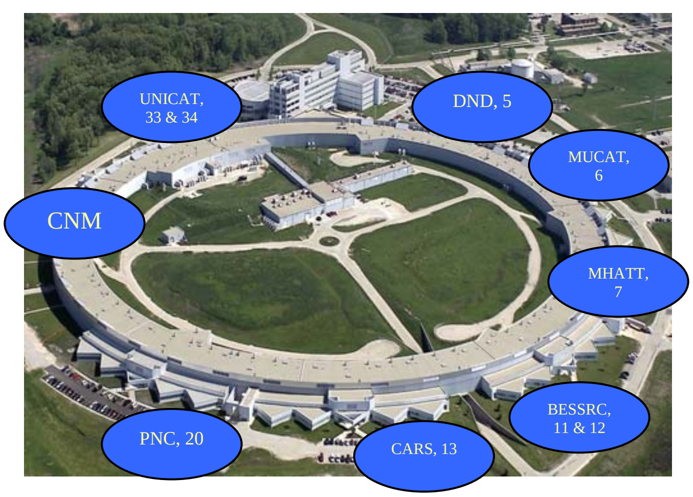
TABLE 1: *In-situ* characterization usage of the APS by beamline for the fiscal years 2004 and 2005. Also shown is time used for *ex-situ* measurements that are closely linked to, and in support of, *In-situ* programs. These statistics were obtained by analyzing beamline schedules and from summaries provided by CAT directors. The usage is presented as a fraction of the general user time available on an APS insertion device beamline each year. These statistics don't include bending magnet beamline usage, grazing incidence SAXS, or liquid scattering experiments.

Many of these experimental protocols depend on considerable off-line access to the specialized equipment for characterization and establishment of processing or growth conditions. In fact, in most cases the Special Purpose instrumentation resides in the last station along a beamline (e.g., an "endstation") to facilitate this access while other experiments are performed in upstream independently operated experimental hutches.

Some of these experiments and techniques require a particular energy for contrast enhancement or to avoid a specific fluorescent effect. Others require full scanning capability of the beamline monochromator to obtain chemical information about the reacting interfaces. Some measurements do not require specific x-ray energy and are often made at a fixed energy. The requirements of the x-ray beam are as diverse as the science represented.

Because experiments that probe two-dimensional structures often require the high brightness at the APS (especially for real-time studies of phenomena), the capabilities for in-situ surface and interface diffraction have been developed primarily on insertion device beamlines. In fact, during the last two years, activity in this research area has represented the equivalent of approximately 3 insertion device beamlines. Even with modest growth projections that take into account new users in areas such as geosciences and electrochemistry, as well as planned hires of scientific staff, the demand for these capabilities at the APS is expected to grow in excess of 4 insertion device beamlines in the near future.

There are also some applications (particularly ex-situ studies) that can utilize APS bending magnet dipole radiation. These include studies of static or slowly varying interfacial systems and measurements that make use of the continuous energy spectrum of dipole radiation. In addition, there are other grazing incidence reflectivity, grazing incidence small angle x-ray scattering, liquid surface scattering and General Purpose scattering capabilities throughout the APS that fall outside the scope of this workshop.



Distribution of Surface and Interface Science around the Advanced Photon Source:

Sector 5 – UHV surface chamber
Sector 6 – UHV surface chamber, thin film deposition
Sector 7 – COBRA
Sector 11 – Electrochemical and geochemical interfaces
Sector 12 – MOCVD, standing waves, electrochemistry, geochemistry, oxidation
Sector 13 – General Purpose surface diffraction
Sector 20 – MBE capable surface xafs, reflectivity, standing wave chamber, COBRA
Sector 33 – UHV chamber/thin film growth, PLD system
Sector 34 – UHV chamber with coherent diffraction

3.2 Staffing of In-situ Efforts

The existing programs at the APS have been primarily funded and supported through the CAT system. For that reason, the APS has few researchers on its staff who are experienced in the relevant experimental techniques. It is however recognized that for outside general users to effectively exploit these capabilities at the APS, state of the art instruments need to be available and operated by experts who are resident at the APS and who work closely with these outside groups. Providing such support is a difficult challenge since these efforts tend to rely heavily on the sophisticated technologies developed in industry, at large research centers and in specialized university laboratories. To date, most successful programs, even those driven by Collaborative Access Teams, have relied heavily on the guidance and expertise of non-affiliated experts.

3.3 Access Modes

As the APS moves away from operations of beamline facilities by traditional Collaborative Access Teams, potential users access the Advanced Photon Source (APS) either as Partner Users or as General Users. Some of the experiments in surface and interface scattering that do not require elaborate or specialized endstation equipment are suitable for General User access. However, the commitment, training and investment to successfully participate in many of these complicated experiments that depend on specialized cells or chambers is much greater than that required for General Users. For some of these, Partner User access is appropriate.

A Partner User is expected to contribute to the facility or user community beyond simply performing good scientific research, as is the objective of a General User. This access mode is sometimes appropriate for developing or operating specialized in-situ growth or processing instrumentation, or developing a new experimental technique. Typically, access to more than 10% of the beam time on a beamline or sector for two years or more would be available for a successful Partner User Proposal. This is consistent with the level of commitment for many of the current activities in this area.

There are limitations associated with both existing access modes. Whereas it is the objective of the APS to make its facilities available to General Users, outside groups who wish to develop new, specialized instrumentation for *in-situ* characterization or processing are often not funded to provide support to other users. Development of many *in-situ* processes requires incorporation of much detailed and sophisticated knowledge from the users' home institutions and, possibly, from external commercial partners. To attract new science and technologies in this area, and remain sensitive to the goal of the APS (as a National User Facility) to make facilities available to the General User community is challenging. In areas that the APS would like to attract intellectual capital and financial investment, it may be necessary to explore new access policies.

3.4 Recommendations

A wide range of exciting and visionary concepts for use of synchrotron radiation to attack problems of both fundamental and technological importance was discussed by the workshop participants. Since many of these concepts are in the early stages of development, the recommendations presented here are based on a conservative survey of existing and planned usage of the APS. The APS should maintain a continued dialogue with the community to help develop forward-looking concepts, and to continually incorporate advances into their strategic and tactical planning. The community should be encouraged, in conjunction with the APS, to generate proposals to develop the resources necessary to exploit these opportunities.

While there were many ideas discussed and many suggestions put forth to enhance the support of the existing and planned research programs, the following recommendations represent the consensus on the critical issues. These recommendations derive ultimately from the desire to exploit scientific opportunities in the area of in-situ surface and interface science. It is believed that implementation of these recommendations will help to ensure the vitality and productivity of this research area. The workshop participants recommend that the APS:

1. **Provide state of the art beamline facilities and infrastructure to support current forefront research efforts, and expand facilities to enable anticipated new opportunities.** There is a general consensus that *in-situ* programs at the APS would benefit from a central facility that would provide a focus for the effort. However, it is unlikely that a single facility could meet the current needs (3 undulator beamlines) and anticipated further demands (one additional undulator beamline) of such a large, diverse community. Additional capacity will be required to meet the needs of this growing community, and distributed capabilities offer the experimental diversity often required. It is important to consider not only the x-ray requirements but also the demands on supporting infrastructure and the need for routine, non-beam access to the processing equipment in developing these plans.
2. **Increase the number of XOR staff scientists whose research encompasses the area of surface and interface scattering.** This will ensure that the research in this area performed at the APS remains at the forefront, that new users will have the support to effectively use powerful capabilities at the APS, and that the user community can be well served.
3. **Establish a formal mechanism to get the advice and recommendations of the research community in the development of these research facilities.** Success in this area is highly dependent on incorporating leading edge technologies and expertise from a variety of sources. It is difficult for any institution to possess all of the relevant expertise in-house. Thus, it is important that the APS be proactive in seeking out guidance and vetting the relevant plans with the expert and extended user community.
4. **Encourage and support user community efforts to develop a proposal for a greenfield facility for materials creation, processing, and in-situ surface and interface and characterization**. Many exciting forefront initiatives in materials creation, processing, and in-situ characterization were highlighted in this workshop. The opportunity to coordinate these activities in a facility uniquely designed to exploit the APS source and advanced x-ray techniques, together with a close relationship with the scientists and

capabilities of the CNM holds great promise for discovery in areas such as interfacial and surface chemistry, fundamental growth processes, and nano-scale sciences.

5. **Develop suitable access modes and policies to encourage strong *in-situ* characterization and processing programs.** Many of the current capabilities at the APS were developed through the successful efforts of Collaborative Access Teams. The engagement of the community of users external to the APS is essential and long-term access based on the scientific and technical merit of the research will facilitate this involvement.

6. **Enable access to other capabilities at ANL.** Users often have needs that cross into other advanced x-ray techniques, or require capabilities that are available or planned at the CNM and in the research divisions of ANL. All users of the APS will benefit from straightforward access to additional preparation and characterization tools available at ANL.

Appendix A
Workshop Program

Thursday, September 8
Building 402 Auditorium

7:30 Registration Open

8:00 Coffee/Continental Breakfast

8:45 Welcome and Statement of Goals

8:50 M. Gibson, *Advanced Photon Source, Argonne National Laboratory*

Overview (Chair: G. Shenoy, APS)

9:00 Surface and Interface Science—Quo Vadis?
J. F. van der Veen, Swiss Light Source

9:40 Uniqueness of Surface Crystallographic Structure Solutions
I. K. Robinson, University of Illinois at Urbana-Champaign

10:10 Coffee

Growth and Processing I (Chair: G. B. Stephenson, Argonne)

10:30 Assembly of Epitaxial Nanostructures on Silicon Surfaces
R. Hull, University of Virginia

11:10 Metal Organic Chemical Vapor Deposition of (Al,In,Ga)N for Solid State Lighting
A. Munkholm, Lumileds

11:30 Study of Nonequilibrium Processes in Pulsed Laser Deposition of Complex Oxides Using Surface X-ray Diffraction
G. Eres, Oak Ridge National Laboratory

11:50 Customizing Oxides and Integrating Them with Semiconductors: Status and Dreams
D. Schlom, Penn State University

12:10 Working Lunch — Access Modes

Frontiers of Interfacial Science (Chair: R. Pindak, NSLS)

1:20 *In-situ* Tribology: What's Really Happening in the Buried Sliding Interface
K. Wahl, Naval Research Laboratory

2:00 Functional Monolayers for Biological Interfaces to Microelectronics
R. J. Hamers, University of Wisconsin, Madison

2:20 Interfacial Dynamics of Polymers and SAMs: Glassy Dynamics, Hierarchical Assembly and the Quest for Perfection
S. Sibener, University of Chicago

2:40 Discussion

Thursday, September 8 (Continued)

Poster Session

2:50 Building 402 Gallery

Self-Organization (Chair: M. Toney, SSRL)

3:50 Quantum Effects on Thin Film Growth, Structure, and Properties
T. Chiang, University of Illinois at Urbana-Champaign

4:10 Structure and Composition Characterization of Self-Assembled Semiconductor Quantum Materials
C-H. Hsu, National Synchrotron Radiation Research Center

4:30 Integrated Modeling and Experimental Studies of Homoepitaxial Thin Film Growth
J. Evans, Ames Laboratory and Iowa State University

4:50 Discussion

5:00 Adjourn to Tours

5:45 Cocktails – Cash Bar, Argonne Guest House

7:00 No-Host Dinner, Argonne Guest House

Friday, September 9, 2005

Building 402 Auditorium

7:30 Registration Open

8:00 Coffee/Continental Breakfast

8:30 Welcome and Summary

Growth and Processing II (Chair: J. Eastman, Argonne)

8:40 Application of Advanced Photon Sources to Multicomponent and Strain-Based Energy Band Engineering of Heterojunction Devices
J. S. Harris, Stanford University

9:20 *In-situ* Synchrotron X-ray Studies of Cu(001) Oxidation
D. Fong, Argonne National Laboratory

9:40 Time-Resolved Studies of Surface Processes on NSLS X21
K. Ludwig, Boston University

10:00 Discussion

10:10 Coffee

Friday, September 9 (Continued)

Real-Space Methods (Chair: S. Brennan, SSRL)

10:30 X-ray Standing Wave Imaging of Atoms at Interfaces
M. J. Bedzyk, Northwestern University

10:50 Atomic-Scale Visualization of Surfaces
P. F. Lyman, University of Wisconsin, Milwaukee

11:10 Thin Film & Substrate Film Interfaces with Sub-Angstrom Resolution using CoBRA
Y. Yacoby, The Hebrew University

11:30 Fullerene on Noble Metals: Interface Structure Solved by X-ray Diffraction
R. Felici, European Synchrotron Radiation Facility

11:50 Discussion

12:00 Working Lunch — Facilities

Complex Interfaces (Chair: N. Sturchio, University of Illinois at Chicago)

1:10 Synchrotron-Based Studies of Environmental Surfaces, Interfaces, and Reactions
G. E. Brown, Jr., Stanford University

1:50 Ion Adsorption Profiles at Mineral–Water Interfaces Probed with Resonant Anomalous X-ray Reflectivity
C. Park, Argonne National Laboratory

2:10 *In-situ* X-ray Diffraction Studies of the Electrode–Solution Interface
N. M. Markovic, Lawrence Berkeley National Laboratory

2:30 CNM Perspective
Stephen Streiffer, Center for Nanoscale Materials, Argonne National Laboratory

2:50 Coffee

Summary and Future Plans

3:00 Discussion

3:30 Adjourn

Appendix B
List of Participants:

First Name	Last Name	Affiliation
Kaveh	Adib	Corning Inc.
Jean-Paul	Allain	ANL/ET
Michael	Bedzyk	Northwestern
Maxim	Boyanov	ANL/ER
Sean	Brennan	SSRL
Gordon	Brown	Stanford U.
Wallis	Calaway	ANL/MSD
Jeffrey G.	Catalano	ANL
Kee-Chul	Chang	ANL/MSD
Yu-Sheng	Chen	U. of Chicago
Tai C.	Chiang	UIUC
Ramana	Chintalapalle	U. Michigan
Yongsoo	Choi	UIC
Shih-Chun	Chung	NSRRC
David	Cookson	APS
Carrie	Crot	UIC
Jeffrey	Eastman	ANL/MSD
Peter	Eng	U. of Chicago
Gyula	Eres	ORNL
Anthony	Escuadro	Northwestern
Paul	Evans	U. Wisc.
James	Evans	Iowa State University
Katherine T.	Faber	Northwestern
Roberto	Felici	ESRF
Paul	Fenter	ANL
Brent	Fiedler	Northwestern
Dillon	Fong	ANL/MSD
John	Freeland	APS
Paul	Fuoss	ANL/MSD
Sanjit	Ghose	U. of Chicago
Murray	Gibson	APS
Dipak	Goswami	Northwestern
Robert	Hamers	Univ of Wisconsin
Ross	Harder	Univ. Of Illinois
James	Harris	Stanford U.

Jan	Hessler	ANL
Hawoong	Hong	UIUC
Chia-Hung	Hsu	NSRRC
Robert	Hull	U. Virginia
Eric	Isaacs	ANL/CNM
Craig	Jeffrey	U. Missouri
Pete	Jemian	UNICAT
Fan	Jiang	ANL/MSD
Christopher	Johnson	ANL
Evguenia	Karapetrova	UNICAT
Denis	Keane	Northwestern
Ishaque	Khan	IIT
Chang-Yong	Kim	Northwestern
Hiroki	Kisu	Canon
Vaibhav	Kohli	Northwestern
Vladimir	Komanicky	ANL/MSD
Charles	Korn	Ben Gurion University
Bernard	Kozioziemski	LLNL
Jeremy	Kropf	ANL/CMT
Ben	Larson	ORNL
Yen-Ru	Lee	UIUC
Myungae	Lee	U. of Chicago
Sang Soo	Lee	UIC
Jui-Ching	Lin	Northwestern
Di-Jia	Liu	ANL/CMT
David	Londono	DuPont
Gabrielle	Long	APS
Karl	Ludwig	Boston University
Paul F.	Lyman	U. Wisc.
Ching	Ma	Northwestern
Beihai	Ma	ANL/ET
Al	Macrander	APS
Bruce	Manning	San Francisco State U.
Nenad	Markovic	ANL/MSD
Christopher	Marshall	ANL
Paul	Miceli	U. Missouri
Dennis	Mills	APS
Habib O.	Moltaji	Carnegie Institution of Washington
Anneli	Munkholm	Lumileds Lighting

Deborah	Myers	ANL/CMT
Kathryn	Nagy	UIC
Diep	Nguyen	Cabot Microelectronics
Christopher	Nicklin	Diamond Light Source
Martin	Nieto	ANL/ET
Zhongwei	Niu	U. South Carolina
Ahmet	Ozcan	Boston University
Changyong	Park	ANL/ER
Amanda	Petford-Long	ANL
Ronald	Pindak	NSLS
Eric	Rexer	ANL/Chemistry
Andrew	Richter	Valparaiso U.
Ian	Robinson	Univ. of Illinois
Philip	Ryan	Ames Lab
Darrell	Schlom	Penn State U.
Mark	Schlossman	UIC
Gopal	Shenoy	APS
Bing	Shi	ANL/MSD
Oleg	Shpyrko	ANL/CNM
Lindsay	Shuller	U. Michigan
Steven	Sibener	U. of Chicago
Frances N.	Skomurski	U. Michigan
Brian	Stephenson	ANL/MSD
Steven	Streiffer	ANL/CNM
Neal	Sturchio	UIC
Sanja	Tepavcevic	UIC
Carol	Thompson	Northern Illinois Univ
Aleksey	Tikhonov	NSLS
Jon	Tischler	ORNL
Michael	Toney	SSRL
King-Long	Tsang	NSRRC
Stefan	Vajda	ANL/Chemistry
J. Friso	van der Veen	Paul Scherrer Institut
John	Vaughey	ANL/CMT
Boyd	Veal	ANL/MSD
Albert	Wagner	ANL
Kathryn	Wahl	NRL
Don	Walko	APS
Ruey-Ven	Wang	ANL/CNM
Didier	Wermeille	MU-CAT

Gerold	Willing	U. Louisville
Huifang	Xu	U. Wisc.
Yizhak	Yacoby	Hebrew University
Yaw-Wen	Yang	NSRRC
Junbing	Yang	ANL/CMT
Rakesh	Yeredla	U. Wisc.
Bilge	Yildiz	ANL/NE
Hoydoo	You	ANL/MSD
Lei	Zhang	DuPont
Nianli	Zhang	U. Wisc.
Zhan	Zhang	ANL/ER
Fan	Zhang	APS
Linjuan	Zhong	ANL/MSD
Manshui	Zhou	UIC
Guangwen	Zhou	ANL/MSD
Paul	Zschack	APS